meso-Hexestrol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.24

Global applicability domain: Inside

Local applicability domain index: 4.84e-01

Confidence level: 5.85e-01

Nearest Neighbors from the Training Set

Image not found
Estrone
Measured: 3.13
Predicted: 3.54

Image not found
Diethylstilbestrol
Measured: 5.07
Predicted: 3.98

Image not found
5-tert-Butyl-2-(3-hydroxycyclohexyl)phenol
Measured: 4.05
Predicted: 3.90

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2-(3-Hydroxycyclohexyl)-5-(2-methylpentan-2-yl)phenol
Measured: 4.82
Predicted: 4.71